

# Strictly and non-strictly positive definite functions on spheres

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## Abstract

Isotropic positive definite functions on spheres play important roles in spatial statistics, where they occur as the correlation functions of homogeneous random fields and star-shaped random particles. In approximation theory, strictly positive definite functions serve as radial basis functions for interpolating scattered data on spherical domains. We review characterizations of positive definite functions on spheres in terms of Gegenbauer expansions and apply them to dimension walks, where monotonicity properties of the Gegenbauer coefficients guarantee positive definiteness in higher dimensions. Subject to a natural support condition, isotropic positive definite functions on the Euclidean space  $\mathbb{R}^3$ , such as Askey's and Wendland's functions, allow for the direct substitution of the Euclidean distance by the great circle distance on a one-, two- or three-dimensional sphere, as opposed to the traditional approach, where the distances are transformed into each other. Completely monotone functions are positive definite on spheres of any dimension and provide rich parametric classes of such functions, including members of the powered exponential, Matérn and generalized Cauchy families. The sine power family permits a continuous parameterization of the roughness of the sample paths of Gaussian processes on spheres. The paper closes with a set of sixteen research problems that provide challenges for future work in mathematical analysis, probability theory and spatial statistics.

**Key words:** completely monotone; covariance localization; fractal index; interpolation of scattered data; isotropic; locally supported; multiquadric; Pólya criterion; radial basis function; random field on a sphere

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# 1 Introduction

For an integer  $k \geq 2$  let  $\mathbb{S}^{k-1} = \{x \in \mathbb{R}^k : \|x\| = 1\}$  denote the unit sphere in the Euclidean space  $\mathbb{R}^k$ , where we write  $\|x\|$  for the Euclidean norm of  $x \in \mathbb{R}^k$ . A function  $h : \mathbb{S}^d \times \mathbb{S}^d \rightarrow \mathbb{R}$  is *positive definite* if

$$\sum_{i=1}^n \sum_{j=1}^n c_i c_j h(x_i, x_j) \geq 0 \quad (1)$$

for all finite systems of pairwise distinct points  $x_1, \dots, x_n \in \mathbb{S}^d$  and constants  $c_1, \dots, c_n \in \mathbb{R}$ . A positive definite function  $h$  is *strictly positive definite* if the inequality in (1) is strict, unless  $c_1 = \dots = c_n = 0$ , and is *non-strictly positive definite* otherwise. The function  $h : \mathbb{S}^d \times \mathbb{S}^d \rightarrow \mathbb{R}$  is *isotropic* if there exists a function  $\psi : [0, \pi] \rightarrow \mathbb{R}$  such that

$$h(x, y) = \psi(\theta(x, y)) \quad \text{for all } x, y \in \mathbb{S}^d, \quad (2)$$

where  $\theta(x, y) = \arccos(\langle x, y \rangle)$  is the great circle or geodesic distance on  $\mathbb{S}^d$  and  $\langle \cdot, \cdot \rangle$  denotes the scalar product in  $\mathbb{R}^{d+1}$ . Thus, an isotropic function depends on its arguments via the great circle distance  $\theta(x, y)$  or, equivalently, the scalar product  $\langle x, y \rangle$  only.

For  $d = 1, 2, \dots$  we write  $\Psi_d$  for the class of the continuous functions  $\psi : [0, \pi] \rightarrow \mathbb{R}$  with  $\psi(0) = 1$  which are such that the associated isotropic function  $h$  in (2) is positive definite. Hence, we may identify the class  $\Psi_d$  with the correlation functions of the mean-square continuous, stationary and isotropic random fields on the sphere  $\mathbb{S}^d$  (Jones, 1963). We write  $\Psi_d^+$  for the class of the continuous functions  $\psi : [0, \pi] \rightarrow \mathbb{R}$  with  $\psi(0) = 1$  such that the isotropic function  $h$  in (2) is strictly positive definite, and we define  $\Psi_d^- = \Psi_d \setminus \Psi_d^+$ .

Recently, there has been renewed interest in the study of positive definite functions on spheres, motivated in part by applications in spatial statistics, where the members of the class  $\Psi_d$  play crucial roles as the correlation functions of isotropic random fields on spheres (Banerjee, 2005; Huang et al., 2011), including the case of star-shaped random particles (Hansen et al., 2011). In a related development in approximation theory, the members of the class  $\Psi_d^+$  arise as radial basis functions for interpolating scattered data on spherical domains (Fasshauer and Schumaker, 1998; Cavoretto and De Rossi, 2010; Le Gia et al., 2010).

In this paper we study the classes  $\Psi_d$  and  $\Psi_d^+$  with particular attention to the practically most relevant case of correlation functions and radial basis functions on a two-dimensional sphere, such as planet Earth. Applications abound, with atmospheric data assimilation and the reconstruction of the global temperature and green house gas concentration records being key examples. As it turns out, odd dimensions are mathematically more tractable, and so it is convenient to consider positive definite functions on three-dimensional spheres, along with their natural restrictions to one- or two-dimensional spheres. Section 2 summarizes related results for isotropic positive definite functions on Euclidean spaces and studies their restrictions to spheres. In Section 3 we review characterizations of strictly and non-strictly positive definite functions on spheres in terms of expansions in ultraspherical or Gegenbauer polynomials, and apply them to dimension walks, where monotonicity properties of the Gegenbauer coefficients in any given dimension guarantee positive definiteness in higher dimensions.

The core of the paper is Section 4, where we supply easily applicable conditions for membership in the classes  $\Psi_d$  and  $\Psi_d^+$ , and use them to derive rich parametric families of correlation functions and radial basis functions on spheres. In particular, compactly supported, isotropic positive definite functions on the Euclidean space  $\mathbb{R}^3$  remain positive definite with the great circle distance on a one-, two- or three-dimensional sphere as argument. Consequently, compactly supported radial basis functions on  $\mathbb{R}^3$ , such as Askey's and Wendland's functions, translate directly

Table 1: Parametric families of correlation functions and radial basis functions on one-, two- and three-dimensional spheres in terms of the great circle distance,  $\theta \in [0, \pi]$ . Here  $c$  is a scale or support parameter,  $\tau$  is a shape parameter, and  $\alpha$  or  $\nu$  is a smoothness parameter, respectively, and we write  $t_+ = \max(t, 0)$  for  $t \in \mathbb{R}$ . The parameter range indicated guarantees membership in the classes  $\Psi_d^+$ , where  $d = 1, 2$  and  $3$ . For details see Section 4.

Family	Analytic expression	Parameter range
Powered exponential	$\psi(\theta) = \exp\left(-\left(\frac{\theta}{c}\right)^\alpha\right)$	$c > 0; \alpha \in (0, 1]$
Matérn	$\psi(\theta) = \frac{2^{\nu-1}}{\Gamma(\nu)} \left(\frac{\theta}{c}\right)^\nu K_\nu\left(\frac{\theta}{c}\right)$	$c > 0; \nu \in (0, \frac{1}{2}]$
Generalized Cauchy	$\psi(\theta) = \left(1 + \left(\frac{\theta}{c}\right)^\alpha\right)^{-\tau/\alpha}$	$c > 0; \alpha \in (0, 1]; \tau > 0$
Multiquadric	$(1 - \tau)^{2c} / (1 + \tau^2 - 2\tau \cos \theta)^c$	$c > 0; \tau \in (0, 1)$
Sine power	$\psi(\theta) = 1 - \left(\sin \frac{\theta}{2}\right)^\alpha$	$\alpha \in (0, 2)$
Spherical	$\psi(\theta) = \left(1 + \frac{1}{2}\frac{\theta}{c}\right)\left(1 - \frac{\theta}{c}\right)_+^2$	$c > 0$
Askey	$\psi(\theta) = \left(1 - \frac{\theta}{c}\right)_+^\tau$	$c > 0; \tau \geq 2$
$C^2$ -Wendland	$\psi(\theta) = \left(1 + \tau\frac{\theta}{c}\right)\left(1 - \frac{\theta}{c}\right)_+^\tau$	$c \in (0, \pi]; \tau \geq 4$
$C^4$ -Wendland	$\psi(t) = \left(1 + \tau\frac{\theta}{c} + \frac{\tau^2-1}{3}\frac{\theta^2}{c^2}\right)\left(1 - \frac{\theta}{c}\right)_+^\tau$	$c \in (0, \pi]; \tau \geq 6$

into locally supported radial basis functions on the sphere. A recent paper by Beatson et al. (2011) provides criteria of Pólya type that guarantee membership in the classes  $\Psi_d^+$ , and we supplement these results in the case of spheres of dimension  $d \leq 7$ . Completely monotone functions are strictly positive definite on spheres of any dimension, and include members of the powered exponential, Matérn and generalized Cauchy families. Some of the key results in the cases of one-, two- and three-dimensional spheres are summarized in Table 1, which complements a similar table in the recent work of Huang et al. (2011).

The paper ends in Section 5, where we discuss challenges for future work from both theoretical and applied perspectives. A collection of sixteen research problems in mathematical analysis, probability theory and statistics offers challenges of diverse difficulty and scope.

## 2 Isotropic positive definite functions on Euclidean spaces

In this expository section, we review basic results about isotropic positive definite functions on Euclidean spaces and study their restrictions to isotropic positive definite functions on spheres.

Recall that a function  $h : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$  is *positive definite* if the inequality (1) holds for all finite systems of pairwise distinct points  $x_1, \dots, x_n \in \mathbb{R}^d$  and constants  $c_1, \dots, c_n \in \mathbb{R}$ . It is *strictly positive definite* if the inequality is strict unless  $c_1 = \dots = c_n = 0$ . The function  $h : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$  is *radial*, *spherically symmetric* or *isotropic* if there exists a function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  such that

$$h(x, y) = \varphi(\|x - y\|) \quad \text{for all } x, y \in \mathbb{R}^d. \quad (3)$$

For an integer  $d \geq 1$  we denote by  $\Phi_d$  the class of the continuous functions  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  with  $\varphi(0) = 1$  such that the function  $h$  in (3) is positive definite. Thus, we may identify the class  $\Phi_d$  with the characteristic functions of spherically symmetric probability distributions, or with the correlation functions of mean-square continuous, stationary and isotropic random fields on  $\mathbb{R}^d$ .

Schoenberg (1938) showed that a function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  belongs to the class  $\Phi_d$  if and only if it is of the form

$$\varphi(t) = \int_{[0, \infty)} \Gamma(d/2) \left( \frac{2}{rt} \right)^{(d-2)/2} J_{(d-2)/2}(rt) dF(r) \quad \text{for } t \geq 0, \quad (4)$$

where  $J$  denotes a Bessel function (Digital Library of Mathematical Functions, 2011, Section 10.2) and  $F$  is a probability measure on  $[0, \infty)$ . The classes  $\Phi_d$  are nonincreasing in  $d$ ,

$$\Phi_1 \supset \Phi_2 \supset \dots \supset \Phi_\infty = \bigcap_{d=1}^{\infty} \Phi_d,$$

with the inclusions being strict, and if  $d \geq 2$  any nonconstant member  $\varphi$  of the class  $\Phi_d$  corresponds to a strictly positive definite function on  $\mathbb{R}^d$  (Sun, 1993, Theorem 3.8). As shown by Schoenberg (1938), the class  $\Phi_\infty$  consists of the functions  $\varphi$  of the form

$$\varphi(t) = \int_{[0, \infty)} \exp(-r^2 t^2) dF(r) \quad \text{for } t \geq 0, \quad (5)$$

where  $F$  is a probability measure on  $[0, \infty)$ .

From the point of view of isotropic random fields, the asymptotic decay of the function  $\varphi$  at the origin determines the smoothness of the associated Gaussian sample path almost surely (Adler, 2009; Gneiting et al., 2011). Specifically, if

$$\varphi(0) - \varphi(t) = \mathcal{O}(t^\alpha) \quad \text{as } t \downarrow 0 \quad (6)$$

for some  $\alpha \in (0, 2]$ , which we refer to as the *fractal index*, the graph of a Gaussian sample path has fractal or Hausdorff dimension  $D = d + 1 - \frac{\alpha}{2}$ . If  $\alpha = 2$ , the sample path is smooth and differentiable and its Hausdorff dimension,  $D$ , equals its topological dimension,  $d$ . If  $\alpha \in (0, 2)$ , the sample path is non-differentiable. Table 2 shows some well known parametric families within the class  $\Phi_\infty$ , namely the powered exponential family (Yaglom, 1987), the Matérn class (Guttorp and Gneiting, 2006) and the generalized Cauchy family (Gneiting and Schlather, 2004), along with the corresponding fractal indices. Table 3 shows compactly supported families within the class  $\Phi_3$  that have been discussed by Wendland (1995) and Gneiting (1999a, 2002).

Yadrenko (1983) pointed out that if  $\varphi$  is a member of the class  $\Phi_k$  for some  $k \geq 2$ , then the function defined by

$$\psi(\theta) = \varphi\left(2 \sin \frac{\theta}{2}\right) \quad \text{for } \theta \in [0, \pi], \quad (7)$$

corresponds to the restriction of the isotropic function  $h(x_i, x_j) = \varphi(\|x_i - x_j\|)$  from  $\mathbb{R}^k \times \mathbb{R}^k$  to  $\mathbb{S}^{k-1} \times \mathbb{S}^{k-1}$ , with the chordal or Euclidean distance expressed in terms of the great circle distance,  $\theta$ , on the sphere  $\mathbb{S}^{k-1}$ . Thus, given any nonconstant member  $\varphi$  of the class  $\Phi_k$ , the function  $\psi$  defined by (7) belongs to the class  $\Psi_{k-1}^+$ .

Various authors have argued in favor of this construction, including Fasshauer and Schumaker (1998), Gneiting (1999a), Narcowich and Ward (2002) and Banerjee (2005), as it readily generates parametric families of isotropic, strictly positive definite functions on spheres and retains the

Table 2: Parametric families of members of the class  $\Phi_\infty$ , where  $K_\nu$  denotes the modified Bessel function of the second kind of order  $\nu$  (Digital Library of Mathematical Functions, 2011, Section 10.2),  $c$  is a scale parameter,  $\alpha$  and  $\nu$  are smoothness parameters, and  $\tau$  is a shape parameter, respectively.

Family	Analytic expression	Parameter range	Fractal index
Powered exponential	$\varphi(t) = \exp\left(-\left(\frac{t}{c}\right)^\alpha\right)$	$c > 0; \alpha \in (0, 2]$	$\alpha \in (0, 2]$
Matérn	$\varphi(t) = \frac{2^{\nu-1}}{\Gamma(\nu)} \left(\frac{t}{c}\right)^\nu K_\nu\left(\frac{t}{c}\right)$	$c > 0; \nu > 0$	$\min(2\nu, 2) \in (0, 2]$
Generalized Cauchy	$\varphi(t) = \left(1 + \left(\frac{t}{c}\right)^\alpha\right)^{-\tau/\alpha}$	$c > 0; \alpha \in (0, 2]; \tau > 0$	$\alpha \in (0, 2]$

Table 3: Parametric families of compactly supported members of the class  $\Phi_3$  with support parameter  $c$  and shape parameter  $\tau$ .

Family	Analytic expression	Parameter range	Fractal index
Spherical	$\varphi(t) = \left(1 + \frac{1}{2}\frac{t}{c}\right)\left(1 - \frac{t}{c}\right)_+^2$	$c > 0$	1
Askey	$\varphi(t) = \left(1 - \frac{t}{c}\right)_+^\tau$	$c > 0; \tau \geq 2$	1
$C^2$ -Wendland	$\varphi(t) = \left(1 + \tau\frac{t}{c}\right)\left(1 - \frac{t}{c}\right)_+^\tau$	$c > 0; \tau \geq 4$	2
$C^4$ -Wendland	$\varphi(t) = \left(1 + \tau\frac{t}{c} + \frac{\tau^2-1}{3}\frac{t^2}{c^2}\right)\left(1 - \frac{t}{c}\right)_+^\tau$	$c > 0; \tau \geq 6$	2

interpretation of scale, support, shape and smoothness parameters. In particular, the mapping (7) from  $\varphi \in \Phi_k$  to  $\psi \in \Psi_{k-1}$  preserves the fractal index, in the sense that

$$\psi(0) - \psi(\theta) = \mathcal{O}(\theta^\alpha) \quad \text{as } \theta \downarrow 0 \quad (8)$$

if  $\varphi$  has fractal index  $\alpha \in (0, 2]$ , as defined in (6). Nevertheless, the approach is of limited flexibility. For example, if  $\varphi \in \Phi_3$  it is readily seen from (4) that the function  $\psi$  defined in (7) does not admit values less than  $\inf_{t>0} t^{-1} \sin t = -0.2127 \dots$ . Furthermore, the mapping  $\theta \mapsto 2 \sin \frac{\theta}{2}$  in the argument of  $\varphi$  in (7), while being essentially linear for small  $\theta$ , is counter to spherical geometry for larger values of the great circle distance, and thus may result in physically unrealistic distortions. In this light, we turn to characterizations and constructions of positive definite functions that operate directly on a sphere.

### 3 Isotropic positive definite functions on spheres

Let  $d \geq 1$  be an integer. As defined in Section 1, the classes  $\Psi_d$  and  $\Psi_d^+$  consist of the functions  $\psi : [0, \pi] \rightarrow \mathbb{R}$  with  $\psi(0) = 1$  which are such that the isotropic function  $h$  in (2) is positive definite and strictly positive definite, respectively. Furthermore, we consider the class  $\Psi_d^- = \Psi_d \setminus \Psi_d^+$  of the non-strictly positive definite functions, and we define

$$\Psi_\infty = \bigcap_{d=1}^{\infty} \Psi_d, \quad \Psi_\infty^+ = \bigcap_{d=1}^{\infty} \Psi_d^+ \quad \text{and} \quad \Psi_\infty^- = \bigcap_{d=1}^{\infty} \Psi_d^-.$$

Schoenberg (1942) noted that the classes  $\Psi_d$  and  $\Psi_\infty$  are convex, closed under products and closed under limits, provided the limit function is continuous. The classes  $\Psi_d^+$  and  $\Psi_\infty^+$  are convex and closed under products, but not under limits.

We proceed to review Schoenberg's (1942) classical representation of the members of the classes  $\Psi_d$  and  $\Psi_\infty$  in terms of ultraspherical or Gegenbauer expansions, along with the associated characterizations of strict positive definiteness in a more recent strand of literature in approximation theory. Towards this end, we require some classical results on orthogonal polynomials (Digital Library of Mathematical Functions, 2011, Section 18.3). Given  $\lambda > 0$  and an integer  $n \geq 0$ , the function  $C_n^\lambda(\cos \theta)$  is defined by the expansion

$$\frac{1}{(1 + r^2 - 2r \cos \theta)^\lambda} = \sum_{n=0}^{\infty} r^n C_n^\lambda(\cos \theta) \quad \text{for } \theta \in [0, \pi], \quad (9)$$

where  $r \in (-1, 1)$ , and  $C_n^\lambda$  is called the ultraspherical or Gegenbauer polynomial of degree  $n$ . For reference later on, we note that  $C_n^\lambda(1) = \Gamma(n + 2\lambda)/(n! \Gamma(2\lambda))$ . If  $\lambda = 0$ , we follow Schoenberg (1942) and set

$$C_n^0(\cos \theta) = \cos(n\theta) \quad \text{for } \theta \in [0, \pi].$$

By equation (3.42) of Askey and Fitch (1969),

$$C_n^\lambda(\cos \theta) = \frac{\Gamma(\nu)}{\Gamma(\lambda)\Gamma(\lambda - \nu)} \sum_{k=0}^{[n/2]} \frac{(n - 2k + \nu)\Gamma(k + \lambda - \nu)\Gamma(n - k + \lambda)}{k!\Gamma(n - k + \nu + 1)} C_{n-2k}^\nu(\cos \theta) \quad (10)$$

whenever  $\lambda > \nu \geq 0$  and  $\theta \in [0, \pi]$ , where the coefficients on the right-hand side are strictly positive. This classical result of Gegenbauer will be used repeatedly in the sequel.

The following theorem summarizes Schoenberg's (1942) characterization of the classes  $\Psi_d$  and  $\Psi_\infty$ , along with the corresponding results of Chen et al. (2003) and Menegatto (1994) for the classes  $\Psi_d^+$  and  $\Psi_\infty^+$ , respectively.

**Theorem 1** (Schoenberg; Chen, Menegatto and Sun). *Let  $d \geq 1$  be an integer.*

(a) *The class  $\Psi_d$  consists of the functions of the form*

$$\psi(\theta) = \sum_{n=0}^{\infty} b_{n,d} \frac{C_n^{(d-1)/2}(\cos \theta)}{C_n^{(d-1)/2}(1)} \quad \text{for } \theta \in [0, \pi], \quad (11)$$

*with nonnegative coefficients  $b_{n,d}$  such that  $\sum_{n=0}^{\infty} b_{n,d} = 1$ . If  $d \geq 2$ , the class  $\Psi_d^+$  consists of the functions in  $\Psi_d$  with the coefficients  $b_{n,d}$  being strictly positive for infinitely many even and infinitely many odd integers  $n$ .*

(b) *The class  $\Psi_\infty$  consists of the functions of the form*

$$\psi(\theta) = \sum_{n=0}^{\infty} b_n (\cos \theta)^n \quad \text{for } \theta \in [0, \pi], \quad (12)$$

*with nonnegative coefficients  $b_n$  such that  $\sum_{n=0}^{\infty} b_n = 1$ . The class  $\Psi_\infty^+$  consists of the functions in  $\Psi_\infty$  with the coefficients  $b_n$  being strictly positive for infinitely many even and infinitely many odd integers  $n$ .*

If  $d = 1$ , Schoenberg's representation (11) reduces to the general form,

$$\psi(\theta) = \sum_{n=0}^{\infty} b_{n,1} \cos(n\theta) \quad \text{for } \theta \in [0, \pi], \quad (13)$$

of a member of the class  $\Psi_1$ , that is, a standardized, continuous positive definite function on the circle. By basic Fourier calculus,

$$b_{0,1} = \frac{1}{\pi} \int_0^\pi \psi(\theta) d\theta \quad (14)$$

and

$$b_{n,1} = \frac{2}{\pi} \int_0^\pi \cos(n\theta) \psi(\theta) d\theta \quad (15)$$

for all integers  $n \geq 1$ . If  $\psi \in \Psi_1^+$ , then  $b_{n,1}$  is strictly positive for infinitely many even and infinitely many odd integers  $n$  (Menegatto, 1995, Theorem 2.2), but the converse is not necessarily true, and a concise characterization of the class  $\Psi_1^+$  remains elusive. If  $d = 2$ , the representation (11) yields the general form,

$$\psi(\theta) = \sum_{n=0}^{\infty} \frac{b_{n,2}}{n+1} P_n(\cos \theta) \quad \text{for } \theta \in [0, \pi], \quad (16)$$

of a member of the class  $\Psi_2$  in terms of the Legendre polynomial  $P_n$  of integer order  $n \geq 0$ . As Bingham (1973) noted, the classes considered here are convex, and so (11), (12), (13) and (16) can be interpreted as Choquet representations.

The general form (12) of the members of the class  $\Psi_\infty$  can be interpreted as a power series in the variable  $\cos \theta$  with nonnegative coefficients. For example, a standard Taylor expansion shows that the function defined by

$$\psi(\theta) = \frac{(1 - \tau)^{2c}}{(1 + \tau^2 - 2\tau \cos \theta)^c} \quad \text{for } \theta \in [0, \pi] \quad (17)$$

admits such a representation if  $c > 0$  and  $\tau \in (0, 1)$ ; furthermore, the coefficients are strictly positive, whence  $\psi$  belongs to the class  $\Psi_\infty^+$ . When  $d = 2$ , the special cases in (17) with the parameter  $c$  fixed at  $\frac{1}{2}$  and  $\frac{3}{2}$  have been known as the inverse multiquadric and the Poisson spline, respectively (Freedman et al., 1997; Cavoretto and De Rossi, 2010). In this light, we refer to (17) as the *multiquadric* family.

The *sine power* function of Soubeyrand et al. (2008),

$$\psi(\theta) = 1 - \left( \sin \frac{\theta}{2} \right)^\alpha \quad \text{for } \theta \in [0, \pi], \quad (18)$$

also admits the representation (12) if  $\alpha \in (0, 2]$ . Moreover, the coefficients are strictly positive if  $\alpha \in (0, 2)$ , whence  $\psi$  belongs to the class  $\Psi_\infty^+$ . The parameter corresponds to the fractal index  $\alpha$  in the relationship (8) and thus parameterizes the roughness of the sample paths of the associated isotropic Gaussian processes on spheres.

The classes  $\Psi_d$  are nonincreasing in  $d \geq 1$ , with the following result revealing details about their structure. The statement in part (a) might be surprising, in that a function that is non-strictly positive definite on the sphere  $\mathbb{S}^d$  cannot be strictly positive definite on a lower-dimensional sphere, including the case  $\mathbb{S}^1$  of the circle.

**Corollary 1.**

- (a) If  $\psi \in \Psi_d^+ \cap \Psi_{d'}$  for positive integers  $d$  and  $d'$ , then  $\psi \in \Psi_{d'}^+$ . Similarly, if  $\psi \in \Psi_d^- \cap \Psi_{d'}$  for positive integers  $d$  and  $d'$ , then  $\psi \in \Psi_{d'}^-$ . In particular,

$$\Psi_\infty = \Psi_\infty^+ \cup \Psi_\infty^-, \quad (19)$$

where the union is disjoint.

- (b) The classes  $\Psi_d^+$  are nonincreasing in  $d$ ,

$$\Psi_1^+ \supset \Psi_2^+ \supset \cdots \supset \Psi_\infty^+ = \bigcap_{d \geq 1} \Psi_d^+,$$

with the inclusions being strict.

- (c) The classes  $\Psi_d^-$  are nonincreasing in  $d$ ,

$$\Psi_1^- \supset \Psi_2^- \supset \cdots \supset \Psi_\infty^- = \bigcap_{d \geq 1} \Psi_d^-,$$

with the inclusions being strict.

*Proof.* In part (a) we use an argument of Narcowich (1995), while our key tool in proving that the inclusions in parts (b) and (c) are strict is Gegenbauer's relationship (10).

- (a) If  $d \geq d'$ , it is trivially true that  $\psi \in \Psi_d^+$  implies  $\psi \in \Psi_{d'}^+$ . If  $d < d'$ , suppose, for a contradiction, that  $\psi \in \Psi_{d'}^-$ . By part (a) of Theorem 1 applied in dimension  $d' \geq 2$ ,  $\psi$  is either an arbitrary even function plus an odd polynomial in  $\cos \theta$ , or an arbitrary odd function plus an even polynomial in  $\cos \theta$ . By Theorem 2.2 of Menegatto (1995) we conclude that  $\psi \in \Psi_1^-$ , for the desired contradiction to the assumption that  $\psi \in \Psi_d^+$ . Thus,  $\psi \in \Psi_{d'}^+$ . The proof of the second claim is analogous, and the statement in (19) then is immediate.
- (b) The inclusion  $\Psi_{d+1}^+ \subseteq \Psi_d^+$  is trivially true. To see that the inclusion is strict, note that by part (a) of Theorem 1 and the relationship (10) any  $\psi \in \Psi_{d+1}^+$  admits a representation of the form (11) with  $b_{n,d}$  being strictly positive for all integers  $n \geq 0$ . However, there are members of the class  $\Psi_d^+$  with  $b_{n,d} = 0$  for at least one integer  $n \geq 0$  (Chen et al., 2003), which thus do not belong to the class  $\Psi_{d+1}^+$ .
- (c) The inclusion  $\Psi_{d+1}^- \subseteq \Psi_d^-$  is immediate from part (a). To demonstrate that the inclusion is strict, we show that if  $n \geq 2$  then the function  $\psi(\theta) = C_n^{(d-1)/2}(\cos \theta)$  belongs to  $\Psi_d^-$  but not to  $\Psi_{d+1}^-$ . For a contradiction, suppose that  $\psi \in \Psi_{d+1}^-$ . Then by the relationship (10),  $\psi$  is of the form (11) with at least two distinct coefficients  $b_{n,d}$  being strictly positive, contrary to the fact that  $\psi$  is an extreme point of the convex class  $\Psi_d$ .  $\square$

The following classical result is a consequence of Schoenberg's representation (11) and the orthogonality properties of the ultraspherical or Gegenbauer polynomials.

**Corollary 2** (Schoenberg). *Let  $d \geq 2$  be an integer. A continuous function  $\psi : [0, \pi] \rightarrow \mathbb{R}$  with  $\psi(0) = 1$  belongs to the class  $\Psi_d$  if and only if*

$$b_{n,d} = \frac{2n + d - 1}{2^{3-d}\pi} \frac{(\Gamma(\frac{d-1}{2}))^2}{\Gamma(d-1)} \int_0^\pi C_n^{(d-1)/2}(\cos \theta) (\sin \theta)^{d-1} \psi(\theta) d\theta \geq 0 \quad (20)$$

for all integers  $n \geq 0$ . Furthermore, the coefficient  $b_{n,d}$  in the Gegenbauer expansion (11) of a function  $\psi \in \Psi_d$  equals the above value.



Interesting related results include Theorem 4.1 of Narcowich and Ward (2002), which expresses the Legendre coefficient  $b_{n,d}$  of a function  $\psi$  of the form (7), where  $k = d+1$ , in terms of the Fourier transform of the respective member  $\varphi$  of the class  $\Phi_{d+1}$ , and Theorem 6.2 of Le Gia et al. (2010), which deduces asymptotic estimates.

We now provide formulas that express the Gegenbauer coefficient  $b_{n,d+2}$  in terms of the coefficients  $b_{n,d}$  and  $b_{n+2,d}$ . In special cases, closely related results were used by Beatson et al. (2011).

**Corollary 3.** *Consider the coefficients  $b_{n,d}$  in the Gegenbauer expansion (11) of the members of the class  $\Psi_d$ .*

(a) *It is true that*

$$b_{0,3} = b_{0,1} - \frac{1}{2}b_{2,1} \quad (21)$$

*and*

$$b_{n,3} = \frac{1}{2}(n+1)(b_{n,1} - b_{n+2,1}) \quad (22)$$

*for all integers  $n \geq 1$ .*

(b) *If  $d \geq 2$ , then*

$$b_{n,d+2} = \frac{(n+d-1)(n+d)}{d(2n+d-1)}b_{n,d} - \frac{(n+1)(n+2)}{d(2n+d+3)}b_{n+2,d} \quad (23)$$

*for all integers  $n \geq 0$ .*

*Proof.* We take advantage of well known recurrence relations for trigonometric functions and Gegenbauer polynomials.

(a) The identity in (21) holds true because  $2(\sin \theta)^2 = 1 - \cos(2\theta)$  for  $\theta \in [0, \pi]$ , so that

$$b_{0,3} = \frac{2}{\pi} \int_0^\pi (\sin \theta)^2 \psi(\theta) d\theta = \frac{1}{\pi} \int_0^\pi (1 - \cos(2\theta)) \psi(\theta) d\theta = b_{0,1} - \frac{1}{2}b_{2,1}.$$

To establish (22), we note that

$$C_n^1(\cos \theta)(\sin \theta)^2 = \sin \theta \sin((n+1)\theta) = \frac{1}{2}(\cos(n\theta) - \cos((n+2)\theta))$$

for  $\theta \in [0, \pi]$ . In view of the formulas (20) and (15) for the Gegenbauer coefficients  $b_{n,3}$  and the Fourier cosine coefficients  $b_{n,1}$ , respectively, the claim follows easily if we integrate the above equality over  $\theta \in [0, \pi]$ .

(b) By equation (18.9.8) of Digital Library of Mathematical Functions (2011),

$$\begin{aligned} C_n^{(d+1)/2}(\cos \theta)(\sin \theta)^2 &= \frac{(n+d-1)(n+d)}{(d-1)(2n+d+1)} C_n^{(d-1)/2}(\cos \theta) \\ &\quad - \frac{(n+1)(n+2)}{(d-1)(2n+d+1)} C_{n+2}^{(d-1)/2}(\cos \theta). \end{aligned}$$

In view of the formula (20) for the Gegenbauer coefficients  $b_{n,d}$ , we establish (23) by integrating the above equality over  $\theta \in [0, \pi]$  and consolidating coefficients.  $\square$

If  $k \geq 1$  is an integer, so that  $d = 2k + 1$  is odd, the recursion (23) allows us to express the Gegenbauer coefficient  $b_{n,d}$  in terms of the Fourier cosine coefficients  $b_{n,1}, b_{n+2,1}, \dots, b_{n+2k,1}$ . For instance,

$$b_{n,5} = \frac{(n+2)(n+3)}{3 \cdot 4} \left( b_{n,1}^* - 2 \frac{n+2}{n+3} b_{n+2,1} + \frac{n+1}{n+3} b_{n+4,1} \right) \quad (24)$$

for all integers  $n \geq 0$ , where  $b_{0,1}^* = 2b_{0,1}$  and  $b_{n,1}^* = b_{n,1}$  if  $n \geq 1$ . Similarly, if  $d = 2k + 2$  is even, we can express the Gegenbauer coefficient  $b_{n,d}$  in terms of the Legendre coefficients  $b_{n,2}, b_{n+2,2}, \dots, b_{n+2k,2}$ . Furthermore, it is possible to relate the Legendre coefficients to the Fourier cosine coefficients, in that, subject to weak regularity conditions,

$$b_{n,2} = \sum_{k=0}^{\infty} c_k^n (b_{n+2k,1}^* - b_{n+2k+1,1}), \quad (25)$$

where

$$c_k^n = \frac{2^{2n}(n!)^2}{(2n)!} \frac{1 \cdot 3 \cdots (2k-1)}{k!} \frac{(n+1) \cdot (n+2) \cdots (n+k)}{(2n+3) \cdot (2n+5) \cdots (2n+2k+1)}$$

for integers  $n \geq 0$  and  $k \geq 0$ , as used in special cases by Huang et al. (2011).

The recursions in Corollary 3 allow for dimension walks, where monotonicity properties of the Fourier cosine or Gegenbauer coefficients in a given dimension guarantee positive definiteness in higher dimensions, as follows.

**Corollary 4.** *Suppose that the function  $\psi : [0, \pi] \rightarrow \mathbb{R}$  is continuous with  $\psi(0) = 1$ . For integers  $d \geq 1$  and  $n \geq 0$ , let  $b_{n,d}$  denote the Fourier cosine and Gegenbauer coefficients (14), (15) and (20) of  $\psi$ , respectively.*

(a) *The function  $\psi$  belongs to the class  $\Psi_3$  if, and only if,  $b_{2,1} \leq 2b_{0,1}$  and  $b_{n+2,1} \leq b_{n,1}$  for all integers  $n \geq 1$ . It belongs to the class  $\Psi_3^+$  if, and only if, furthermore, the inequality is strict for infinitely many even and infinitely many odd integers.*

(b) *If  $d \geq 2$ , the function  $\psi$  belongs to the class  $\Psi_{d+2}$  if, and only if,*

$$b_{n+2,d} \leq \frac{2n+d+3}{2n+d-1} \frac{(n+d-1)(n+d)}{(n+1)(n+2)} b_{n,d} \quad (26)$$

*for all integers  $n \geq 0$ . It belongs to the class  $\Psi_{d+2}^+$  if, and only if, furthermore, the inequality is strict for infinitely many even and infinitely many odd integers.*

(c) *If  $d \geq 2$ , the function  $\psi$  belongs to the class  $\Psi_{d+2}^+$  if  $b_{n+2,d} \leq b_{n,d}$  for all integers  $n \geq 0$ .*

*Proof.* Parts (a) and (b) are immediate from Corollaries 2 and 3 in concert with Theorem 1; part (c) then follows from part (b).  $\square$

## 4 Criteria for positive definiteness and applications

In this section we provide easily applicable tests for membership in the classes  $\Psi_d$  and  $\Psi_d^+$  and apply them to construct rich parametric families of correlation functions and radial basis functions on spheres.

## 4.1 Locally supported strictly positive definite functions on two- and three-dimensional spheres

There are huge computational savings in the interpolation of scattered data on spheres if the strictly positive definite function used as the correlation or radial basis function admits a simple closed form, and is supported on a spherical cap. Thus, various authors have sought such functions (Schreiner, 1997; Fasshauer and Schumaker, 1998; Narcowich and Ward, 2002), with particular emphasis on the practically most relevant case of the two-dimensional sphere.

The following result of Lévy (1961) constructs a positive definite function on the circle from a positive definite function on the real line, in the form of a compactly supported member of the class  $\Phi_1$ . Here and in the following, we write  $\varphi_{[0,\pi]}$  for the restriction of a function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  to the interval  $[0, \pi]$ . Essentially identical results can be found in Sasvári (1994, Exercise 1.10.25) and Wood (1995).

**Theorem 2 (Lévy).** *Suppose that the function  $\varphi \in \Phi_1$  is such that  $\varphi(t) = 0$  for  $t \geq \pi$ . Then the restriction  $\psi = \varphi_{[0,\pi]}$  belongs to the class  $\Psi_1$ .*

On the two-dimensional sphere, a particularly simple way of constructing a locally supported member of the corresponding class  $\Psi_2^+$  is to take a compactly supported member of the class  $\Phi_3$ , such as any of the functions in Table 3, and apply Yadrenko's recipe (7). If  $\varphi \in \Phi_3$  is such that  $\varphi(t) = 0$  for  $t \geq a$ , where  $a \in (0, \pi)$ , then the function  $\psi$  in (7) belongs to the class  $\Psi_2^+$  and satisfies  $\psi(\theta) = 0$  for  $\theta \geq 2 \arcsin \frac{a}{2}$ . However, the approach is subject to the problems described in Section 2, in that the use of the chordal distance may result in physically unrealistic representations.

Perhaps surprisingly, the following result shows that compactly supported, isotropic positive definite functions on the Euclidean space  $\mathbb{R}^3$  remain positive definite with the great circle distance on a one-, two- or three-dimensional sphere as argument. Thus, they can be used either with the chordal distance or with the great circle distance as argument.

**Theorem 3.** *Suppose that the function  $\varphi \in \Phi_3$  is such that  $\varphi(t) = 0$  for  $t \geq \pi$ . Then the restriction  $\psi = \varphi_{[0,\pi]}$  belongs to the class  $\Psi_3^+$ .*

*Proof.* If the function  $\varphi \in \Phi_3$  is such that  $\varphi(t) = 0$  for  $t \geq \pi$ , the Fourier cosine coefficient (15) of its restriction  $\psi = \varphi_{[0,\pi]}$  can be written as

$$b_{n,1} = \frac{2}{\pi} \int_0^\pi \cos(n\theta) \psi(\theta) d\theta = \frac{1}{\pi} \int_{\mathbb{R}} \cos(nt) \phi(t) dt = 2\hat{\phi}(n)$$

for all integers  $n \geq 1$ . Here, the function  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  is defined by  $\phi(t) = \varphi(|t|)$  for  $t \in \mathbb{R}$ , and  $\hat{\phi}(u) = \frac{1}{2\pi} \int_{\mathbb{R}} \cos(ut) \phi(t) dt$  denotes the inverse Fourier transform of  $\phi$  evaluated at  $u \in \mathbb{R}$ . Similarly,  $b_{0,1} = \hat{\phi}(0)$ . By equation (36) of Gneiting (1998a) in concert with the Paley-Wiener theorem (Paley and Wiener, 1934), the function  $\hat{\phi}(u)$  is strictly decreasing in  $u \geq 0$ . Thus, the sequence  $b_{n,1}$  is strictly decreasing in  $n \geq 1$ ; furthermore,  $b_{2,1} = 2\hat{\phi}(2) < 2\hat{\phi}(0) = 2b_{0,1}$ . By part (a) of Corollary 4, we conclude that  $\psi \in \Psi_3^+$ .  $\square$

Theorem 3 permits us to use any of the functions in Table 3 with support parameter  $c \leq \pi$  as a correlation function or radial basis function with the spherical or great circle distance on the sphere  $\mathbb{S}^d$  as argument, where  $d \leq 3$ . This gives rise to flexible parametric families of locally supported

members of the class  $\Psi_d^+$ , where  $d \leq 3$ , that admit particularly simple closed form expressions. A first example is the *spherical* family,

$$\psi(\theta) = \left(1 + \frac{1}{2} \frac{\theta}{c}\right) \left(1 - \frac{\theta}{c}\right)_+^2 \quad \text{for } \theta \in [0, \pi], \quad (27)$$

which derives from the family (34) in the class  $\Phi_3$  that serves as a popular correlation model in geostatistics (Gneiting, 1999c). Huang et al. (2011, Section 3.2) showed that the function  $\psi$  in (27) is in the class  $\Psi_2^+$  if  $c \leq \pi$ ; Theorem 3 yields the stronger result that  $\psi \in \Psi_3^+$  if  $c \leq \pi$ .

Using families of compactly supported members of the class  $\Phi_3$  introduced and discussed by Askey (1973), Wendland (1995) and Gneiting (1999a), Theorem 3 confirms that the truncated power function

$$\psi(\theta) = \left(1 - \frac{\theta}{c}\right)_+^\tau \quad \text{for } \theta \in [0, \pi] \quad (28)$$

belongs to the class  $\Psi_3^+$  if  $\tau \geq 2$  and  $c \in (0, \pi)$ , as shown previously by Beatson et al. (2011). If smoother functions are desired, the Wendland function

$$\psi(\theta) = \left(1 + \tau \frac{\theta}{c}\right) \left(1 - \frac{\theta}{c}\right)_+^\tau \quad \text{for } \theta \in [0, \pi] \quad (29)$$

is in  $\Psi_3^+$  if  $\tau \geq 4$  and  $c \in (0, \pi)$ ; similarly, the function defined by

$$\psi(t) = \left(1 + \tau \frac{\theta}{c} + \frac{\tau^2 - 1}{3} \frac{\theta^2}{c^2}\right) \left(1 - \frac{\theta}{c}\right)_+^\tau \quad \text{for } \theta \in [0, \pi] \quad (30)$$

belongs to the class  $\Psi_3^+$  if  $\tau \geq 6$  and  $c \in (0, \pi)$ .

In atmospheric data assimilation, locally supported isotropic positive definite functions play important roles in the distance-dependent filtering of spatial covariance estimates on planet Earth (Hamill et al., 2001; Buehner and Charron, 2007). The traditional construction in this literature relies on the Gaspari and Cohn (1999) function,

$$\varphi_{GC}(t) = \begin{cases} 1 - \frac{20}{3}t^2 + 5t^3 + 8t^4 - 8t^5, & 0 \leq t \leq \frac{1}{2}, \\ \frac{1}{3}t^{-1}(8t^2 + 8t - 1)(1 - t)^4, & \frac{1}{2} \leq t \leq 1, \\ 0, & t \geq 1, \end{cases}$$

which belongs to the class  $\Phi_3$ , along with all functions of the form  $\varphi(t) = \varphi_{GC}(t/c)$ , where  $c > 0$  is a constant. Yadrenko's construction (7) then yields the localization function

$$\psi_1(\theta) = \varphi_{GC}\left(\frac{\sin \frac{\theta}{2}}{\sin \frac{c}{2}}\right) \quad \text{for } \theta \in [0, \pi], \quad (31)$$

which is a member of the class  $\Psi_2^+$  with support  $[0, c]$ . Theorem 3 suggests a natural alternative, in that, for every  $c \in [0, \pi]$ , the function defined by

$$\psi_2(\theta) = \varphi_{GC}\left(\frac{\theta}{c}\right) \quad \text{for } \theta \in [0, \pi] \quad (32)$$

is also a member of the class  $\Psi_2^+$  with support  $[0, c]$ . Clearly,  $\psi_2(\theta) > \psi_1(\theta)$  for  $\theta \in (0, c)$ , as illustrated in Figure 1, where  $c = \frac{\pi}{2}$ . This suggests that  $\psi_2$  might be a more effective localization function than the traditional choice,  $\psi_1$ , in operational data assimilation. Similar comments might apply to covariance tapers in spatial statistics, as proposed and applied by Furrer et al. (2006) and Kaufman et al. (2008), among others.

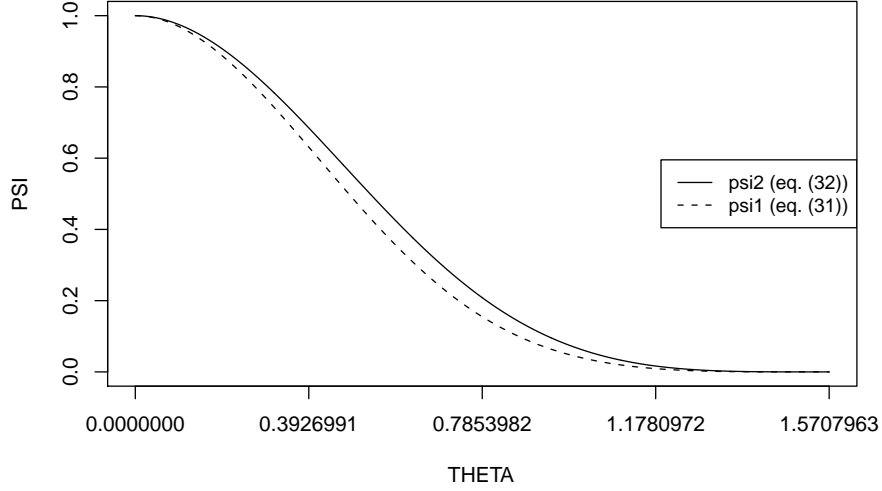


Figure 1: The Gaspari and Cohn (1999) localization function with Euclidean or chordal distance as argument ( $\psi_1$ ; equation (31)), and with spherical or great circle distance as argument ( $\psi_2$ ; equation (32)), respectively, where  $c = \frac{\pi}{2}$ . While both functions are members of the class  $\Psi_2^+$  and have support  $[0, c]$ , we note that  $\psi_2(\theta) > \psi_1(\theta)$  for  $\theta \in (0, c)$ , which suggests that  $\psi_2$  might be a more effective localization function.

## 4.2 Criteria of Pólya type

Criteria of Pólya type provide simple sufficient conditions for positive definiteness by imposing convexity conditions on a candidate function and/or its higher derivatives. Gneiting (2001) reviews and develops Pólya criteria on Euclidean spaces; in what follows, we are concerned with analogues on spheres that complement the recent work of Beatson et al. (2011).

The following theorem summarizes criteria developed by Wood (1995), Gneiting (1998b) and Beatson et al. (2011) in the case of the circle  $\mathbb{S}^1$ .

**Theorem 4.** *Suppose that the function  $\psi : [0, \pi] \rightarrow \mathbb{R}$  is continuous, nonincreasing and convex with  $\psi(0) = 1$  and  $\int_0^\pi \psi(\theta) d\theta \geq 0$ . Then  $\psi$  belongs to the class  $\Psi_1$ . It belongs to the class  $\Psi_1^+$ , unless it is piecewise linear.*

Our next result is a Pólya criterion that applies on spheres  $\mathbb{S}^d$  of dimension  $d \leq 3$ . Its proof relies on the subsequent lemmas, the first of which is well known.

**Theorem 5.** *Suppose that  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  is a continuous function with  $\varphi(0) = 1$ ,  $\lim_{t \rightarrow \infty} \varphi(t) = 0$  and a continuous derivative  $\varphi'$  such that  $-\varphi'(t^{1/2})$  is convex for  $t > 0$ . Then the restriction  $\psi = \varphi_{[0, \pi]}$  belongs to the class  $\Psi_3^+$ .*

To give an example, we may conclude from Theorem 5 that the truncated power function (28) with shape parameter  $\tau \geq 2$  belongs to the class  $\Psi_3^+$  for all values of the support parameter  $c > 0$ , including the case  $c > \pi$ , in which it is supported globally.

**Lemma 1.** *Let  $d \geq 1$  be an integer. Suppose that  $C$  is a subset of a Euclidean space, and let  $P$  be a Borel probability measure on  $C$ . If  $\psi_c$  belongs to the class  $\Psi_d$  for every  $c \in C$ , then the function*

$\psi$  defined by

$$\psi(\theta) = \int_C \psi_c(\theta) dP(c) \quad \text{for } \theta \in [0, \pi]$$

belongs to the class  $\Psi_d$ , too. If furthermore  $\psi_c$  belongs to  $\Psi_d^+$  for every  $c$  in a set of positive  $P$ -measure, then  $\psi$  belongs to the class  $\Psi_d^+$ .

**Lemma 2.** For all  $c > 0$ , the function defined by

$$\psi_c(\theta) = \left(1 + \frac{1}{2} \frac{\theta}{c}\right) \left(1 - \frac{\theta}{c}\right)_+^2 \quad \text{for } \theta \in [0, \pi] \quad (33)$$

belongs to the class  $\Psi_3^+$ .

*Proof.* By Theorem 3, the function  $\psi_c$  belongs to the class  $\Psi_3^+$  if  $c \leq \pi$ . If  $c \geq \pi$ , equations (14) and (15) yield the Fourier cosine coefficients

$$b_{0,1} = \frac{\pi}{16c^3} (8c^3 - 6\pi c^2 + \pi^3) \quad \text{and} \quad b_{1,1} = \frac{3}{2c^3} (4 + 2c^2 - \pi^2).$$

For  $k = 1, 2, \dots$ , we find that

$$b_{2k,1} = \frac{3\pi^2}{8c^3} \frac{1}{k^2}$$

and

$$b_{2k+1,1} = \frac{3}{2c^3} \left( \frac{2c^2 - \pi^2}{(2k+1)^2} - 2 \frac{2c^2 - \pi^2 - 2}{(2k+1)^4} \right).$$

Thus,  $b_{2,1} < 2b_{0,1}$  and  $b_{2k+2,1} < b_{2k,1}$  for all integers  $k \geq 1$ . As regards the odd Fourier cosine coefficients, let  $k \geq 1$  and note that

$$b_{2k+1,1} - b_{2k+3,1} = \frac{12}{c^3} \frac{k+1}{(2k+1)^4 (2k+3)^4} g(k),$$

where

$$g(k) = (2c^2 - \pi^2)(16k^4 + 44k^3 + 88k^2 + 48k + 9) + 8(4k^2 + 8k + 5) > 0,$$

whence  $b_{2k+3,1} < b_{2k+1,1}$  for all integers  $k \geq 0$ . Therefore, we conclude from part (a) of Corollary 4 that  $\psi_c$  belongs to the class  $\Psi_3^+$  for  $c \geq \pi$ .  $\square$

*Proof of Theorem 5.* By Theorem 3.1 of Gneiting (1999c), the function  $\varphi$  admits a representation of the form

$$\varphi(t) = \int_{(0,\infty)} \varphi_c(t) dF(c) \quad \text{for } t \geq 0,$$

where  $\varphi_c$  is defined by

$$\varphi_c(t) = \left(1 + \frac{1}{2} \frac{t}{c}\right) \left(1 - \frac{t}{c}\right)_+^2 \quad \text{for } t \geq 0, \quad (34)$$

and  $F$  is a probability measure on  $(0, \infty)$ . Therefore, the restriction  $\psi = \varphi_{[0,\pi]}$  is of the form

$$\psi(\theta) = \int_{(0,\infty)} \psi_c(\theta) dF(c) \quad \text{for } \theta \in [0, \pi],$$

where  $\psi_c$  is defined by (33). By Lemma 2, the function  $\psi_c$  belongs to the class  $\Psi_3^+$  for all  $c > 0$ , and so we conclude from Lemma 1 that  $\psi$  is in  $\Psi_3^+$ .  $\square$

Our next theorem is a slight generalization of the key result in Beatson et al. (2011). In analogy to the corresponding results on Euclidean spaces in Gneiting (1999c), the case  $n = 1$  yields a more concise, but less general, criterion than Theorem 5.

**Theorem 6.** *Let  $n \leq 3$  be a positive integer. Suppose that  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  is a continuous function with  $\varphi(0) = 1$ ,  $\lim_{t \rightarrow \infty} \varphi(t) = 0$  and a derivative  $\varphi^{(n)}$  of order  $n$  such that  $(-1)^n \varphi^{(n)}(t)$  is convex for  $t > 0$ . Then the restriction  $\psi = \varphi_{[0, \pi]}$  belongs to the class  $\Psi_{2n+1}^+$ .*

In a recent *tour de force*, Beatson et al. (2011) demonstrate the following remarkable result about the truncated power function, which is the key to proving Theorem 6.

**Lemma 3** (Beatson, zu Castell and Xu). *Let  $n \leq 3$  be a positive integer, and suppose that  $c \in (0, \pi)$ . Then the function defined by*

$$\psi_{c,n}(\theta) = \left(1 - \frac{\theta}{c}\right)_+^{n+1} \quad \text{for } \theta \in [0, \pi] \quad (35)$$

*belongs to the class  $\Psi_{2n+1}^+$ .*

The next lemma concerns the case  $c > \pi$ , in which the truncated power function (35) is supported globally.

**Lemma 4.** *For all integers  $n \geq 1$  and all real numbers  $c \geq \pi$ , the function  $\psi_{c,n}$  in (35) belongs to the class  $\Psi_\infty^+$ .*

*Proof.* By a convolution argument due to Fuglede (Hjorth et al., 1998, p. 272), the function  $\psi_{\pi,0}(\theta) = 1 - \frac{\theta}{\pi}$  belongs to the class  $\Psi_\infty$ . As the class  $\Psi_\infty$  is convex and closed under products, we see that if  $n \geq 0$  is an integer and  $c \geq \pi$  then

$$\psi_{c,n}(\theta) = \left( \left(1 - \frac{\pi}{c}\right) + \frac{\pi}{c} \psi_{\pi,0}(\theta) \right)^{n+1} \quad \text{for } \theta \in [0, \pi],$$

whence  $\psi_{c,n}$  is in the class  $\Psi_\infty$ , too. By a straightforward direct calculation, the Fourier cosine coefficients of  $\psi_{c,1}$  and  $\psi_{c,2}$  are strictly positive for all  $c \geq \pi$ . Therefore, by Theorem 1 of Xu and Cheney (1992) and the fact that the class  $\Psi_1^+$  is closed under products, the function  $\psi_{c,n}$  is in the class  $\Psi_1^+$  for all integers  $n \geq 1$  and all  $c \geq \pi$ . Using part (a) of Corollary 1, we conclude that  $\psi_{c,n} \in \Psi_\infty^+$  for all integers  $n \geq 1$  and all  $c \geq \pi$ .  $\square$

*Proof of Theorem 6.* By Theorem 3.1 of Gneiting (1999c), the function  $\varphi$  admits a representation of the form

$$\varphi(t) = \int_{(0, \infty)} \varphi_{c,n}(t) \, dF(c) \quad \text{for } t \geq 0,$$

where the function  $\varphi_{c,n} : [0, \infty) \rightarrow \mathbb{R}$  is defined by

$$\varphi_{c,n}(t) = \left(1 - \frac{t}{c}\right)_+^{n+1} \quad \text{for } t \geq 0$$

and  $F$  is a probability measure on  $(0, \infty)$ . Therefore, the restriction  $\psi = \varphi_{[0, \pi]}$  is of the form

$$\psi(\theta) = \int_{(0, \infty)} \psi_{c,n}(\theta) \, dF(c) \quad \text{for } \theta \in [0, \pi],$$

where  $\psi_{c,n}$  is defined by (35). By Lemmas 3 and 4 the function  $\psi_{c,n}$  belongs to the class  $\Psi_{2n+1}^+$  for all  $c > 0$ . Therefore, we conclude from Lemma 1 that  $\psi$  is in  $\Psi_{2n+1}^+$ , too.  $\square$

Beatson et al. (2011) conjectured that the statement of Lemma 3 holds for all integers  $n \geq 1$ . In view of Lemma 4, if their conjecture is true, the statement of Theorem 6 holds for all integers  $n \geq 1$ , too, with the proof being unchanged.

It is interesting to observe that Theorem 6 is a stronger result than Theorem 1.3 of Beatson et al. (2011), in that it does not impose any support conditions on the candidate function  $\psi$ . In contrast, Theorem 1.3 of Beatson et al. (2011) requires  $\psi$  to be locally supported. Such an assumption is also made in the following result.

**Theorem 7.** *Let  $c \in (0, \pi)$ , and let  $\psi : [0, \pi] \rightarrow \mathbb{R}$  be a continuous function with  $\psi(0) = 1$  and  $\psi(\theta) = 0$  for  $\theta \geq c$ .*

- (a) *Let  $k \geq 1$  be an integer. Suppose that  $\psi$  has derivatives of all orders up to  $2k$  on  $(0, \pi)$  and define*

$$\eta_1(\theta) = \left( -\frac{d}{du} \right)^k \psi(\sqrt{u}) \Big|_{u=\theta^2}.$$

*If there exists an  $\alpha \geq \frac{1}{2}$  such that*

$$\eta_2(\theta) = \left( -\frac{d}{d\theta} \right)^{k-1} [-\eta_1'(\theta^\alpha)]$$

*is convex on  $(0, \pi)$ , then  $\psi$  belongs to the class  $\Psi_1$ .*

- (b) *Let  $k \geq 0$  be an integer. Suppose that  $\psi$  has derivatives of all orders up to  $2k + 1$  on  $(0, \pi)$  and define*

$$\eta_1(\theta) = \left( -\frac{d}{du} \right)^k \psi(\sqrt{u}) \Big|_{u=\theta^2}.$$

*If there exists an  $\alpha \geq \frac{1}{2}$  such that*

$$\eta_2(\theta) = \left( -\frac{d}{d\theta} \right)^k [-\eta_1'(\theta^\alpha)]$$

*is convex on  $(0, \pi)$ , then  $\psi$  belongs to the class  $\Psi_3^+$ .*

*Proof.* We first prove part (a). Define the function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  by  $\varphi(t) = \psi(t)$  for  $t \in [0, \pi]$  and  $\varphi(t) = 0$  for  $t \geq \pi$ . By Proposition 2.1 of Gneiting (2001), where we set  $l = 0$ ,  $\varphi$  admits a representation of the form

$$\varphi(t) = \int_{(0, \infty)} \varphi_k\left(\frac{t}{c}\right) dF(c) \quad \text{for } t \geq 0, \quad (36)$$

where the function  $\varphi_k : [0, \infty) \rightarrow \mathbb{R}$  is a certain member of the class  $\Phi_1$  that is supported on the unit interval  $[0, 1]$ , and  $F$  is a probability measure on  $(0, \infty)$ . However, as  $\varphi(t) = 0$  for  $t \geq \pi$ , the probability measure  $F$  must be concentrated on the interval  $(0, \pi]$ . Therefore, the candidate function  $\psi$  admits a representation of the form

$$\psi(\theta) = \int_{(0, \pi]} \psi_c(\theta) dF(c) \quad \text{for } \theta \in [0, \pi], \quad (37)$$



where  $\psi_c$  denotes the restriction of the mapping  $t \mapsto \varphi_k(\frac{t}{c})$  to the interval  $[0, \pi]$ . By Theorem 2, the function  $\psi_c$  belongs to the class  $\Psi_1$  for all  $c \in (0, \pi]$ . Thus, we conclude from Lemma 1 that  $\psi$  belongs to the class  $\Psi_1$ .

The proof of part (b) is identical, except that we set  $l = 1$  in Proposition 2.1 of Gneiting (2001), the function  $\varphi_k$  in (36) is a certain member of the class  $\Phi_3$  that is supported on the unit interval, and by Theorem 3 the function  $\psi_c$  in (37) belongs to the class  $\Psi_3^+$  for all  $c \in (0, \pi]$ . Therefore, we conclude from Lemma 1 that  $\psi$  belongs to the class  $\Psi_3^+$ .  $\square$

When  $k = 0$  in part (b) of Theorem 7, the function  $\psi_c$  in the representation (37) is of the specific form (27), and the resulting criterion reduces to a weaker version of Theorem 5. The stronger statement in Theorem 5 depends on the fact that  $\psi_c \in \Psi_3^+$  for all  $c > 0$ , including the case  $c > \pi$  in which  $\psi_c$  is supported globally. This property depends on the asymptotic linearity of the function  $\varphi_0$  in (36) at the origin, as reflected by its fractal index,  $\alpha = 1$ . By Proposition 2.1 of Gneiting (2001), the function  $\varphi_k$  in the crucial representation (36) has fractal index  $\alpha = 2$  if  $k \geq 1$ , in both part (a) and part (b), and thus the condition that  $c \in (0, \pi]$  is essential for the membership of the corresponding function  $\psi_c$  in any of the classes  $\Psi_d$ , as will become evident in Section 4.4.

### 4.3 Completely monotone functions

A function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  is completely monotone if it possesses derivatives  $\varphi^{(k)}$  of all orders with  $(-1)^k \varphi^{(k)}(t) \geq 0$  for all integers  $k \geq 0$  and all  $t > 0$ . Our next result shows that the restrictions of completely monotone functions belong to the class  $\Psi_\infty^+$ .

**Theorem 8.** *Suppose that the function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  is completely monotone with  $\varphi(0) = 1$  and not constant. Then the restriction  $\psi = \varphi_{[0, \pi]}$  belongs to the class  $\Psi_\infty^+$ .*

*Proof.* Let  $a > 0$  and consider the truncated power function (35). By Lemma 4,  $\psi_{n/a, n}$  belongs to the class  $\Psi_\infty^+$  for all sufficiently large integers  $n$ . Hence, the function  $\psi_a$  defined by

$$\psi_a(\theta) = e^{-a\theta} = \lim_{n \rightarrow \infty} \psi_{n/a, n}(\theta) \quad \text{for } \theta \in [0, \pi]$$

belongs to the class  $\Psi_\infty$ , too. By Theorem 5,  $\psi_a \in \Psi_3^+$ , which in view of part (a) of Corollary 1 implies that  $\psi_a \in \Psi_\infty^+$ . Now suppose that the function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  satisfies the conditions of the theorem. Invoking Bernstein's Theorem, we see that  $\varphi$  admits a representation of the form

$$\varphi(t) = \int_{[0, \infty)} e^{-at} dF(a) \quad \text{for } t \geq 0,$$

where  $F$  is a probability measure on  $[0, \infty)$ . Therefore, the restriction  $\psi = \varphi_{[0, \pi]}$  is of the form

$$\psi(\theta) = \int_{[0, \infty)} e^{-a\theta} dF(a) = \int_{[0, \infty)} \psi_a(\theta) dF(a) \quad \text{for } \theta \in [0, \pi].$$

Since  $\varphi$  is not constant,  $F$  has mass away from the origin. As  $\psi_a$  is in the class  $\Psi_\infty^+$  for all  $a > 0$ , we conclude from Lemma 1 that  $\psi$  belongs to the class  $\Psi_\infty^+$ .  $\square$

Miller and Samko (2001) present a wealth of examples of completely monotone functions, which thus can serve as correlation functions or radial basis functions on spheres of any dimension.

## 4.4 Necessary conditions

The next result states conditions that prohibit membership in the class  $\Psi_1$ , and therefore in any of the classes  $\Psi_d$ . Heuristically, the common motif can be paraphrased as follows:

If a positive definite function admits a certain degree of smoothness at the origin, it admits the same degree of smoothness everywhere.

The conditions in parts (a) through (d) of the following theorem can be interpreted as formal descriptions of circumstances under which this overarching principle is violated. Part (a) corresponds to a well-known result in the theory of characteristic functions, parts (b) and (c) are due to Wood (1995) and Gneiting (1998b), respectively, and part (d) rests on a result of Devinatz (1959).

**Theorem 9.** *Suppose that the function  $\psi : [0, \pi] \rightarrow \mathbb{R}$  can be represented as the restriction  $\psi = \phi|_{[0, \pi]}$  of an even and continuous function  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  that satisfies any of the following conditions.*

- (a) *For some integer  $k \geq 1$  the derivative  $\phi^{(2k)}(0)$  exists, but  $\phi$  fails to be  $2k$  times differentiable on  $(0, \pi)$ .*
- (b) *For some integer  $k \geq 1$ , the function  $\phi$  is  $2k - 1$  times continuously differentiable on  $[-\pi, \pi]$  with  $\phi^{(2k-1)}(\pi) \neq 0$  and  $|\phi^{(2k-1)}(t)| \leq b_1 |t|^{\beta_1}$  for some  $b_1 > 0$  and  $\beta_1 > 0$ , and is  $2k + 1$  times continuously differentiable on  $[-\pi, 0) \cup (0, \pi]$  with  $|\phi^{(2k+1)}(t)| \leq b_2 |t|^{-\beta_2}$  for some  $b_2 > 0$  and  $\beta_2 \in (1, 2)$ .*
- (c) *For some integer  $k \geq 1$ , the function  $\phi$  is  $2k$  times differentiable on  $[-\pi, \pi]$  with  $\phi^{(j)}(\pi) \neq 0$  for some odd integer  $j$ , where  $1 \leq j \leq 2k - 1$ .*
- (d) *The function  $\phi$  is analytic and not of period  $2\pi$ .*

Then  $\psi$  does not belong to the class  $\Psi_1$ .

In particular, as we will see in the examples in the next section, if a function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  is strictly positive and strictly decreasing, admits a relationship of the form (6) for some  $\alpha \in (0, 2]$  at the origin, and furthermore is such that the restriction  $\psi = \varphi|_{[0, \pi]}$  belongs to the class  $\Psi_1$ , then necessarily  $\alpha \leq 1$ .

## 4.5 Examples

We now apply the criteria of Sections 4.3 and 4.4 to study parametric families of globally supported correlation functions and radial basis functions on spheres. In doing so, we think of  $a > 0$  or  $c > 0$  as a decay or support parameter, of  $\alpha > 0$  or  $\nu > 0$  as a smoothness parameter, and of  $\tau > 0$  as a shape parameter.

First we consider the families in Table 2, namely the powered exponential, Matérn and generalized Cauchy classes. For the parameter values stated in Table 2 these families serve as isotropic correlation functions on Euclidean spaces, where the argument is the Euclidean distance. We now investigate whether they can serve as isotropic correlation functions with spherical or great circle distance on  $\mathbb{S}^d$  as argument, thereby supplementing and completing the corresponding results of Huang et al. (2011) in the case  $d = 2$ .

In Examples 1 and 2 the results and proofs do not depend on the scale parameter  $c > 0$ , and so we only discuss the smoothness parameter  $\alpha$  or  $\nu$ , respectively.

*Example 1* (powered exponential family). The members of the powered exponential family are of the form

$$\psi(\theta) = \exp\left(-\left(\frac{\theta}{c}\right)^\alpha\right) \quad \text{for } \theta \in [0, \pi]. \quad (38)$$

If  $\alpha \leq 1$ , a straightforward application of Theorem 8 shows that  $\psi \in \Psi_\infty^+$ . If  $\alpha > 1$ , we see from parts (b) and (c) of Theorem 9 that  $\psi$  does not belong to the class  $\Psi_1$ , where part (b) applies when  $\alpha \in (1, 2)$ , and part (c) when  $\alpha \geq 2$ , both using  $k = 1$ . Therefore, if  $\alpha > 1$  then  $\psi$  does not belong to any of the classes  $\Psi_d$ .

*Example 2* (Matérn family). The members of the Matérn family can be written as

$$\psi(\theta) = \frac{2^{\nu-1}}{\Gamma(\nu)} \left(\frac{\theta}{c}\right)^\nu K_\nu\left(\frac{\theta}{c}\right) \quad \text{for } \theta \in [0, \pi], \quad (39)$$

where  $K_\nu$  denotes the modified Bessel function of the second kind of order  $\nu$ , as defined in Digital Library of Mathematical Functions (2011, Section 10.2). If  $\nu = n + \frac{1}{2}$ , where  $n \geq 0$  is an integer, then  $\psi$  equals the product of  $\exp(-\theta/c)$  and a polynomial of degree  $n$  in  $\theta$ . In particular, if  $\nu = \frac{1}{2}$  then  $\psi(\theta) = \exp(-\theta/c)$  for  $\theta \in [0, \pi]$ . If  $\nu = \frac{3}{2}$ , then

$$\psi(\theta) = \left(1 + \frac{\theta}{c}\right) \exp\left(-\frac{\theta}{c}\right) \quad \text{for } \theta \in [0, \pi],$$

and if  $\nu = \frac{5}{2}$  then

$$\psi(\theta) = \left(1 + \frac{\theta}{c} + \frac{1}{3} \frac{\theta^2}{c^2}\right) \exp\left(-\frac{\theta}{c}\right) \quad \text{for } \theta \in [0, \pi].$$

Responding to questions in Sections 3.3.1 and 3.3.4 of Huang et al. (2011), we now seek conditions under which the Matérn function  $\psi$  in (39) is strictly or non-strictly positive definite with spherical distance as argument.

We first show that if  $\nu \leq \frac{1}{2}$  then  $\psi$  belongs to the class  $\Psi_\infty^+$ . Towards this end, we note from Theorem 5 of Miller and Samko (2001) that if  $\nu \leq \frac{1}{2}$  the function  $\phi_1 : \mathbb{R} \rightarrow \mathbb{R}$  defined by  $\phi_1(t) = \exp(t)t^\nu K_\nu(t)$  for  $t \geq 0$  is completely monotone. By Theorem 1 of Miller and Samko (2001) the function  $\phi_0 : \mathbb{R} \rightarrow \mathbb{R}$  defined by  $\phi_0(t) = \exp(-t)\phi_1(t) = t^\nu K_\nu(t)$  for  $t \geq 0$  is completely monotone, too. In view of Theorem 8 this proves our claim.

Next we demonstrate that if  $\nu > \frac{1}{2}$  then  $\psi$  does not belong to the class  $\Psi_1$ , and thus neither to any of the classes  $\Psi_d$ . If  $\nu \in (\frac{1}{2}, 1)$ , this follows from an application of the estimates in Section 10.31 of Digital Library of Mathematical Functions (2011) to part (b) of Theorem 9, where  $k = 1$ ,  $\beta_1 = 2\nu - 1$  and  $\beta_2 = 2\nu - 3$ . If  $\nu \geq 1$ , we apply part (c) of Theorem 9, where  $k = 1$ . The details are tedious but straightforward, and we omit them.

In our next example the results do not depend on the scale parameter  $c > 0$  and the shape parameter  $\tau > 0$ , and so we discuss the smoothness parameter  $\alpha$  only.

*Example 3* (generalized Cauchy family). The members of the generalized Cauchy family are of the form

$$\psi(\theta) = \left(1 + \left(\frac{\theta}{c}\right)^\alpha\right)^{-\tau/\alpha} \quad \text{for } \theta \in [0, \pi]. \quad (40)$$

If  $\alpha \leq 1$ , a straightforward application of Theorem 8 shows that  $\psi$  is a member of the class  $\Psi_\infty^+$ . However, if  $\alpha > 1$  the function  $\psi$  in (40) does not belong to the class  $\Psi_1$ . If  $\alpha \in (1, 2)$ , this is evident from part (b) of Theorem 9, where  $k = 1$ ,  $\beta_1 = \alpha - 1$  and  $\beta_2 = \alpha - 3$ ; if  $\alpha \geq 2$  we apply part (c) of Theorem 9, where also  $k = 1$ .

In the context of isotropic random fields and random particles, the smoothness properties of the associated random surface are governed by the behavior of the correlation function at the origin. Specifically, if a function  $\psi \in \Psi_2$  admits the relationship (8) for some  $\alpha \in (0, 2]$ , the corresponding Gaussian sample path on the two-dimensional sphere has fractal or Hausdorff dimension  $3 - \frac{\alpha}{2}$  almost surely, as shown and described more explicitly by Hansen et al. (2011). In this sense, the results in the above examples are restrictive, in that the smoothness parameter needs to satisfy  $\alpha \leq 1$  or  $\nu \leq \frac{1}{2}$ , respectively. For parametric families of correlation functions that admit the full range of viable Hausdorff dimensions, we refer to the sine power family (18) of Soubeyrand et al. (2008) and the convolution construction in Section 4.3 of Hansen et al. (2011). Alternatively, Yadrenko's construction (7) can be applied to any of the parametric families in Table 2.

In our final example it is convenient to work with the shape parameter  $\tau \geq 1$  and the inverse scale parameter  $r > 0$ , where small values correspond to slowly decaying correlations.

*Example 4* (Bessel family). The members of the Bessel family are analytic functions of the form

$$\psi(\theta) = \Gamma(\tau/2) \left( \frac{2}{r\theta} \right)^{(\tau-2)/2} J_{(\tau-2)/2}(r\theta) \quad \text{for } \theta \in [0, \pi], \quad (41)$$

where  $J$  denotes a Bessel function. Their relevance stems from Schoenberg's representation (4) of the members of the class  $\Phi_d$  in terms of the function in (41), where  $\tau = d$ . As a consequence, the analytic continuation of  $\psi$  to a function  $\varphi : [0, \infty) \rightarrow \mathbb{R}$  belongs to the class  $\Phi_d$  if and only if  $\tau \geq d$ , irrespectively of the value of the scale parameter  $r > 0$ .

We now investigate whether the function  $\psi$  belongs to the class  $\Psi_d$ , starting with the case  $\tau = 1$ , in which (41) reduces to

$$\psi(\theta) = \cos(r\theta) \quad \text{for } \theta \in [0, \pi].$$

This function  $\psi$  can be extended to an analytic function  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  with shortest period  $2\pi/r$ . If  $r = 1$ , then  $\psi$  belongs to the class  $\Psi_\infty^-$ ; if  $r = n$  where  $n \geq 2$  is an integer it belongs to the class  $\Psi_1^- \setminus \Psi_2^-$ , based on arguments in analogy to those in the proof of part (c) of Corollary 1. For non-integer values of the scale parameter  $r > 0$ , part (d) of Theorem 9 implies that  $\psi(\theta) = \cos(r\theta)$  does not belong to the class  $\Psi_1$ .

Similarly, we see from part (d) of Theorem 9 that if  $\tau > 1$  then the function  $\psi$  in (41) does not belong to the class  $\Psi_1$ , irrespectively of the value of  $r > 0$ . Thus, it does not belong to any of the classes  $\Psi_d$ , as shown in Section 3.3 of Huang et al. (2011) in the particular case  $\tau = 3$  and  $d = 2$ .

## 5 Challenges for future work

In this paper, we have reviewed and developed characterizations and constructions of positive definite functions on spheres, and we have applied them to provide rich parametric classes of such functions.

Some of the key results in the practically most relevant cases of one-, two- and three-dimensional spheres are summarized in Table 1. Whenever required, the closure properties of the classes of the positive definite or strictly positive definite functions offer additional flexibility. For example, while all entries in Table 1 yield nonnegative correlations only, we can easily model negative correlations, by using convex sums or products of an entry in the table with a Legendre function of the form  $\psi(\theta) = C_n^{(d-1)/2}(\cos \theta)/C_n^{(d-1)/2}(1)$ , including the case  $\psi(\theta) = \cos \theta$  that arises when  $n = 1$ , irrespectively of the dimension  $d$ .

An important construction principle that we have only touched upon here is spherical convolution, which has been used by Wood (1995), Schreiner (1997), Estrade and Istas (2010) and Hansen et al. (2011) to construct positive definite functions on spheres. For example, if we consider an indicator function  $k(\theta) = \mathbb{1}(\theta \leq r)$  on the two-dimensional sphere, where  $r \in (0, \frac{\pi}{2}]$  is a cut-off parameter, spherical self-convolution yields the member of the class  $\Psi_2$  given by

$$\psi(\theta) = \frac{1}{\pi(1 - \cos r)} \left( \pi - \arccos(\cos \theta \csc^2 r - \cot^2 r) - 2 \cos r \arccos(\csc \theta \cos r \csc r - \cot \theta \cot r) \right) \mathbb{1}(\theta \leq 2r) \quad \text{for } \theta \in [0, \pi],$$

as shown in the appendix of Tovchigrechko and Vakser (2001). In the same setting, Estrade and Istas (2010) develop a recursive formula that yields closed form expressions for the members of the class  $\Psi_d$  that arise from the self-convolution of uniform kernels on  $d$ -dimensional spheres. Hansen et al. (2011) apply the convolution approach to derive a parametric family within the class  $\Psi_2^+$  that admits the full range of viable Hausdorff dimensions for the associated Gaussian and Gaussian-related random fields.

Despite substantial advances in the study of positive definite and strictly positive definite functions on spheres, many interesting and important questions remain open. I will thus close the paper with a set of research problems, which aim to stimulate future research in mathematical analysis, probability theory and spatial statistics. The problems vary in scope and difficulty, range from harmonic analysis to statistical methodology, and include what appear to be tedious but routine questions, such as Problem 2, along with well known major challenges, such as Problem 1 and Problems 14 through 16, which have been under scrutiny for decades.

The first eight problems are of an analytic character and concern the characterization and breadth of the classes  $\Psi_d$  and  $\Psi_d^+$ , respectively.

*Problem 1.* Provide a concise characterization of the class  $\Psi_1^+$  of the strictly positive definite functions on the circle in terms of their Fourier cosine coefficients. Despite recent progress by Chen et al. (2003) and Sun (2005), and related advances for strictly positive definite functions on the real line (Derrien, 2010), the challenge is substantial, and a persuasive solution remains elusive.

*Problem 2.* For integers  $k \geq 1$  and  $n \geq 0$ , find the coefficients  $a_{n,1}, \dots, a_{n,k}$  in the general formula

$$b_{n,2k+1} = \sum_{i=0}^k a_{n,k} b_{n+2i,1}$$

for the Gegenbauer coefficient  $b_{n,2k+1}$  of a function  $\psi \in \Psi_{2k+1}$  in terms of its Fourier cosine coefficients  $b_{n,1}, b_{n+2,1}, \dots, b_{n+2k,1}$ , of which equations (22) and (24) are the first two instances. Similarly, find the coefficients in the general formula for the Gegenbauer coefficient  $b_{n,2k+2}$  in terms of the Legendre coefficients  $b_{n,2}, b_{n+2,2}, \dots, b_{n+2k,2}$ .

We now let  $\Psi_d^c$  denote the class of the functions  $\psi \in \Psi_d$  with  $\psi(\theta) = 0$  for  $\theta \geq c$ , where  $d \geq 1$  is an integer and  $c \in (0, \pi]$ . If  $c < \pi$ , the corresponding correlation function or radial basis function has local support. Similarly, we let  $\Phi_d^c$  denote the class of the functions  $\varphi \in \Phi_d$  with  $\varphi(t) = 0$  for  $t \geq c$ , where  $d \geq 1$  is an integer and  $c > 0$ .

*Problem 3.* Using the notation just introduced,  $\Psi_d^\pi$  is the class of the functions  $\psi \in \Psi_d$  with  $\psi(\pi) = 0$ , and  $\Phi_d^\pi$  is the class of the functions  $\varphi \in \Phi_d$  such that  $\varphi(t) = 0$  if  $t \geq \pi$ . Theorems 2 and 3 express the fact that

$$\Phi_d^\pi \subseteq \Psi_d^\pi \tag{42}$$

when  $d = 1$  and  $d = 3$ , respectively, and these inclusions are critical to the constructions in Section 4. Does the relationship (42) hold true for all integers  $d \geq 1$ ? I have not been able to find a counterexample, nor have I made progress towards a proof. A positive answer would reap immediate benefits, such as far-reaching generalizations of Theorem 6 and Theorem 7.

*Problem 4.* For an integer  $d \geq 1$  and  $c \in (0, \pi]$ , find

$$a_d^c = \inf_{\psi \in \Psi_d^c} [-\psi''(0)]. \quad (43)$$

As hinted at in Section 4.1, this is a problem of applied interest when  $d = 2$ . In atmospheric data assimilation, locally supported isotropic correlation functions are used for the distance-dependent reduction of global scale covariance estimates in ensemble Kalman filter settings (Hamill et al., 2001; Buehner and Charron, 2007). In this context, it is desirable to use a member of the class  $\Psi_2^c$  with minimal curvature at the origin, as formalized by the optimization problem in (43). By Theorem 2 and Theorem 3,

$$a_d^c \leq \inf_{\varphi \in \Phi_d^c} [-\varphi''(0)] = \frac{1}{c^2} \frac{4}{d} j_{(d-2)/2}^2 \quad (44)$$

when  $d = 1$  and  $d = 3$ , respectively, where  $j_\nu$  denotes the first positive zero of the Bessel function  $J_\nu$ . The right-hand equality in (44) holds true for all integers  $d \geq 1$  and all  $c > 0$  (Ehm et al., 2004, Section 5).

*Problem 5.* For an integer  $d \geq 1$  and  $c \in (0, \pi]$ , find the *Turán constant* of a spherical cap of radius  $c$  on the sphere  $\mathbb{S}_d$ . In other words, find

$$\sup_{\psi \in \Psi_d^c} \left[ \int_{\mathbb{S}^d} \psi(\theta(x, y)) \, dy \right],$$

where  $x$  is an arbitrary point on  $\mathbb{S}^d$  and the integral is with respect to the Haar measure. When  $d = 1$ , the problem has been resolved in a strand of literature that includes the works of Stechkin (1972), Gorbachev (2001) and Ivanov and Ivanov (2010). Extant generalizations to higher dimensions apply to convex bodies in Euclidean spaces or to the torus (Révész, 2011), but not to spheres, and so the case  $d \geq 2$  remains open.

*Problem 6.* For an integer  $d \geq 1$ ,  $c \in (0, \pi]$  and  $\theta \in (0, c)$ , find

$$b_d^c(\theta) = \sup_{\psi \in \Psi_d^c} \psi(\theta).$$

When  $d = 1$ , this pointwise version of Turán's problem that has been studied by Arestov et al. (2003), Kolountzakis and Révész (2006) and Ivanov and Ivanov (2010). I am not aware of any results in dimension  $d \geq 2$ , except that lower bounds on  $b_d^c(\theta)$  become available from existing lower bounds in the analogous problem on Euclidean spaces (Ehm et al., 2004) together with Theorem 3 and Yadrenko's construction (7).

*Problem 7.* What are the smoothness properties of the members of the class  $\Psi_d$ ? In the Euclidean case, the members of the class  $\Phi_d$  admit a derivative of order  $[(d-1)/2]$  on  $(0, \infty)$ , where  $[c]$  denote the greatest integer less than or equal to  $c$ , and this is the best estimate possible (Gneiting, 1999b). In the case of spheres, a natural conjecture is that the members of the class  $\Psi_d$  admit a derivative of order  $[(d-1)/2]$  on the open interval  $(0, \pi)$ , and that this is the best estimate possible. In this context, it is of interest to recall from the representation (12) that the members of the class  $\Psi_\infty$  admit an absolutely convergent power series expansion in the variable  $\cos \theta$ , and thus have derivatives of any order on  $(0, \pi)$ .

*Problem 8.* When does the isotropic positive definite function (2) that is represented by a member  $\psi$  of the class  $\Psi_d$  admit a spherical convolution representation in the sense of Schreiner (1997) and Hansen et al. (2011)? If a convolution root exists, can it be taken to be real-valued and isotropic? If  $\psi(\theta) = 0$  for  $\theta \geq c$ , can we find a convolution root that is supported on a spherical cap of radius  $\frac{c}{2}$ ? Ehm et al. (2004) have answers to analogous questions for positive definite functions on Euclidean spaces, many of which are surprising.

Next we state open questions about the parameter spaces for the truncated power family, the generalized sine power family, and the quartic exponential model used by the Berkeley Earth Surface Temperature project.

*Problem 9.* It is tempting to conjecture that if  $c \in (0, \pi)$  then the truncated power function (28) belongs to the class  $\Psi_d$  if and only if  $\tau \geq \frac{1}{2}(d+1)$ . If  $d = 1$ , it is easy to see that the statement is true. Beatson et al. (2011) proved the sufficiency of the condition when  $d = 3, 5$ , and  $7$ , and conjectured it to be sufficient for all odd integers  $d \geq 1$ . Similarly, I conjecture that if  $c \in (0, \pi)$  then the locally supported functions (29) and (30) belong to the class  $\Psi_d$  if and only if  $\tau \geq \frac{1}{2}(d+5)$  and  $\tau \geq \frac{1}{2}(d+9)$ , respectively. Note that if the inclusion (42) holds true in any given dimension  $d$ , then results of Askey (1973), Golubov (1981), Wendland (1995) and Gneiting (1999a) imply the sufficiency of the aforementioned conditions.

*Problem 10.* A natural generalization of the sine power family (18) of Soubeyrand et al. (2008) takes the form

$$\psi(\theta) = 1 - \left( \sin \frac{\pi \theta}{2c} \right)^\alpha \mathbb{1}(\theta \leq c) \quad \text{for } \theta \in [0, \pi]. \quad (45)$$

In addition to the smoothness parameter  $\alpha \in (0, 2]$ , the generalized sine power family admits a scale or support parameter  $c > 0$ ; if  $c < \pi$ , it is locally supported. For what values of  $\alpha \in (0, 2]$  and  $c > 0$  does the generalized sine power function (45) belong to the class  $\Psi_d$ ? As the class  $\Psi_\infty$  does not admit locally supported members, the answer will depend delicately on the dimension  $d$ . The criteria in Section 4 apply, and the results in Pasenchenko (1996) and Gneiting (2000) in concert with Yadrenko's construction (7) can provide sufficient conditions.

*Problem 11.* The key component of the Berkeley Earth Surface Temperature project (Rohde et al., 2011) correlation model on planet Earth is isotropic, depending on spherical distance as

$$\psi(\theta) = \exp \left( - \sum_{i=1}^4 c_i \theta^i \right) \quad \text{for } \theta \in [0, \pi].$$

For what values of the parameter vector  $(c_1, c_2, c_3, c_4)'$  does this function belong to the class  $\Psi_2$ ? In particular, do the values fitted by Rohde et al. (2011, page 11) provide a valid correlation function on the two-dimensional sphere? Unfortunately, the fitted function does not satisfy the assumptions of Theorem 5, nor does part (b) of Theorem 7 apply, as  $\psi$  is globally supported.

The next two problems relate to the fractal index and the sample path properties of Gaussian and Gaussian-related random fields.

*Problem 12.* When  $d = 2$ , Hansen et al. (2011) prove and illustrate that if a function  $\psi \in \Psi_d$  has fractal index  $\alpha \in (0, 2]$ , as reflected by the relationship (8), then any suitably defined, nontrivial Gaussian sample path on a  $d$ -dimensional sphere has fractal or Hausdorff dimension  $d + 1 - \frac{\alpha}{2}$ . Prove this result for spheres of any dimension  $d \geq 1$ .

*Problem 13.* In the case of Euclidean spaces, Abelian and Tauberian theorems relate the behavior of a correlation function at the origin to that of its Fourier transform at infinity (Leonenko and Olenko,

1991; Stein, 1999). Find general analogues on the sphere that relate the behavior of a member of the class  $\Psi_d$  at the origin to the asymptotic decay of the Gegenbauer coefficients  $b_{n,d}$  in (20) as  $n \rightarrow \infty$ . In particular, what asymptotic behavior is associated with a given fractal index  $\alpha \in (0, 2]$ ? In dimension  $d = 1$ , the broad principle is that the fractal index  $\alpha \in (0, 2)$  corresponds to Fourier coefficients  $b_{n,1}$  decaying like  $n^{-\alpha-1}$ , though the details are intricate (Boas, 1967a,b; Binmore and Stratton, 1969; Wolfe, 1973; Chan, 1985). The recursions in Corollary 3 and the results and tools of Malyarenko (2004) and zu Castell and Filbir (2005) seem relevant here.

We close with challenges in spatial and spatio-temporal statistics, where non-isotropic and non-stationary correlation models on spheres are in strong demand, with the isotropic correlation functions discussed in this paper serving as building blocks for these more complex models.

*Problem 14.* The class  $\Psi_d$  can be identified with the class of the correlation functions of the mean-square continuous, stationary and isotropic real-valued random fields on the sphere  $\mathbb{S}^d$ . However, in many cases of practical interest random fields are vector-valued, comprising, for example, multiple environmental, geophysical or meteorological or variables on planet Earth. It is thus of great interest to characterize the corresponding classes of matrix-valued isotropic correlation functions, find analogues of Cramér’s theorem in the Euclidean case, and identify flexible parametric families of such functions. While Yadrenko’s construction (7) generalizes readily and can be applied to the multivariate Matérn family (Gneiting et al., 2010), or to other matrix-valued correlation functions on Euclidean spaces, approaches that operate directly on a sphere are preferable (Jun, 2011).

*Problem 15.* Processes observed on spheres are frequently non-isotropic, with the topography of planet Earth (Gagnon et al., 2006), total column ozone (Stein, 2007) and error fields from global numerical weather prediction models (Weaver and Courtier, 2001; Wu et al., 2002) being examples. It is therefore desirable to develop non-isotropic stochastic process models on spherical domains, similar to the development of non-stationary and non-isotropic correlation models on Euclidean spaces, such as the space deformation technique of Sampson and Guttorp (1992), the stochastic volatility model of Huang et al. (2011) and parametric approaches (Paciorek and Schervish, 2006; Schlather, 2010). On spherical domains, several approaches have emerged, including ramifications of the space deformation technique (Das, 2000), methods using expansions in spherical harmonics Stein (2007), approaches based on differential operators and nested stochastic partial differential equations (Jun and Stein, 2008; Bolin and Lindgren, 2011), and the approach of Katzfuss (2011, Section 4.3) that builds on the work of Paciorek and Schervish (2006) and covariance tapering. Typically observed deviations from isotropy include dependencies of covariance structures on latitudes, with theory being provided by Hitczenko and Stein (2012).

*Problem 16.* Frequently, the temporal development of a process observed on a sphere is also of interest, so that the process needs to be modeled on the sphere cross time. Nevertheless, the literature on the corresponding correlation structures is sparse, with the work of Jun and Stein (2007) being a notable exception.

The challenges in these problems are complementary, thus calling for the development of simultaneously multivariate, non-stationary and spatio-temporal stochastic process models on the sphere, along with statistical methodology for model fitting and model choice. A promising recent development in this direction is the stochastic partial differential equations approach of Lindgren et al. (2011).



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